MESOSCOPIC QUANTUM CIRCUIT THEORY TO

PERSISTENT CURRENT AND COULOMB BLOCKADE *

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Abstract

The quantum theory for mesoscopic electric circuit is briefly described. The uncertainty relation for electric charge and current modifies the tranditional Heisenberg uncertainty relation. The mesoscopic ring is regarded as a pure L-design, and the persistent current is obtained explicitly. The Coulomb blockade phenomenon appears when applying to the pure C-design.

Owning to the dramatic achievement in nanotechnology, there have been many studies on mesoscopic physics [1]. In present talk I briefly demonstrate a quantum mechanical theory for mesoscopic electric circuits based on the fact that electronic charge takes discrete values [2]. As the application of this approach, the persistent current on a mesoscopic ring and the Coulomb blockade phenomena are formulated from a new point of view, about which some details are presented. Most importantly, it is a physical realization of the deformation of quantum mechanics studied considerably by other authors in mathematical physics.

I. QUANTIZED CIRCUIT WITH CHARGE DISCRETENESS

In order to taken into account the discreteness of electronic charge. we must impose that the eigenvalues of the self-adjoint operator $\hat{q}$ (electric charge) take discrete values [2], i.e. $\hat{q}|q> = nq_e|q>$ ($n \in \mathbf{Z}$, $q_e = 1.602 \times 10^{-19}$ coulomb). Since the spectrum of charge is discrete, the inner product in charge representation will be a sum instead of the usual integral and the electric current operator $\hat{P}$ will be defined by the discrete derivatives [3] $\nabla_{q_e}, \overline{\nabla}_{q_e}$. Thus for the mesoscopic quantum electric circuit one will have a finite-difference Schrödinger equation [2]. The uncertainty relation for electric charge and current modifies the tranditional Heisenberg uncertainty relation, namely,

$$\Delta\hat{q} \cdot \Delta\hat{P} \geq \frac{\hbar}{2}(1 + \frac{q_e^2}{\hbar^2} < \hat{H}_0 >). \tag{1}$$

where $\hat{H}_0 = -\frac{\hbar^2}{2}\nabla_{q_e}\overline{\nabla}_{q_e} = -\frac{\hbar^2}{2q_e}(\nabla_{q_e} - \overline{\nabla}_{q_e})$. The Hamiltonian of quantum LC-design in the presence of exterior magnetic flux reads

$$\hat{H} = -\frac{\hbar^2}{2q_e L}(D_{q_e} - \overline{D}_{q_e}) + \frac{1}{2C}\hat{q}^2 + \varepsilon\hat{q} \tag{2}$$

where L and C stand for the inductance and the capacity of the circuit respectively, ε represents the voltage of an adiabatic aource, and the covariant discrete derivatives are defined by

$$D_{q_e} := e^{-\frac{q_e}{\hbar}\phi} \frac{\hat{Q} - e^{i\frac{q_e}{\hbar}\phi}}{q_e}, \quad \overline{D}_{q_e} := e^{\frac{q_e}{\hbar}\phi} \frac{e^{-i\frac{q_e}{\hbar}\phi} - \hat{Q}^+}{q_e}, \qquad (3)$$

where $\hat{Q} := e^{iq_e\hat{p}/\hbar}$ is a minimum 'shift operator' with the property $\hat{Q}^+|n> = e^{i\alpha_{n+1}}|n + 1>$ ($\alpha'_n s$ are undetermined phases). The hamiltonian (2) is covariant under the gauge transformation, $\hat{G}D_{q_e}\hat{G}^{-1} = D'_{q_e}$, $\hat{G}\overline{D}_{q_e}\hat{G}^{-1} = \overline{D}'_{q_e}$ where $\hat{G} := e^{-i\beta\frac{\hat{q}}{\hbar}}$ and the gauge field ϕ transforms as $\phi \to \phi' = \phi - \beta$. The ϕ plays the role of the exterioral magnetic flux threading the circuit.

II. QUANTUM L-DESIGN AND PERSISTENT CURRENT

Now we study the Schrödinger equation for a pure L-design in the presence of magnetic flux,

$$-\frac{\hbar^2}{2q_e L}(D_{q_e} - \overline{D}_{q_e})|\psi> = E|\psi> . \qquad (4)$$

Because its eigenstates can be simultaneous eigenstates of $\hat{p}$, eq.(4) is solved by the eigenstate $|p> = \sum_{n\in \mathbf{Z}} \kappa_n e^{inq_e p/\hbar}|n>$ ($\kappa_n := \exp(i\sum_{j=1}^n \alpha_j)$). The energy spectrum is easily calculated as

$$E(p, \phi) = \frac{2\hbar}{q_e^2} \sin^2\left(\frac{q_e}{2\hbar}(p - \phi)\right) \qquad (5)$$

which has oscillatory property with respect to ϕ or p. Differing from the usual classical pure L-design, the energy of a mesoscopic quantum pure L-design can not be large than $2\hbar/q_e^2$. Clearly, the lowest energy states are those states with $p = \phi + nh/q_e$, then the eigenvalues of the electric current (i.e. $\frac{1}{L}\hat{P}$) of ground state can be obtained [2]. The electric current on a mesoscopic circuit of pure L-design is not null in the presence of a magnetic flux (except $\phi = nh/q_e$). This is a pure quantum characteristic. The persistent current in a mesoscopic L-design is an observable quantity periodically depending on the flux ϕ. Because a mesoscopic metal ring is a natural pure L-design, the formula we obtained is valid for persistent current in a single mesoscopic ring [4]. One can easily calculate the

inductance of mesoscopic metal ring, $L = 8\pi r(\frac{1}{2}\ln\frac{8r}{a} - 1)$ where r is the radius of the ring and a is the radius of the metal wire. Then the formula for persistent current is

$$I(\phi) = \frac{\hbar}{8\pi r(\frac{1}{2}\ln\frac{8r}{a} - 1)q_e}\sin(\frac{q_e}{\hbar}\phi). \tag{6}$$

Differing from the conventional formulation of the persistent current on the basis of quantum dynamics for electrons, our formulation presented a method from a new point of view. Formally, the $I(\phi)$ we obtained is a sine function with periodicity of $\phi_0 = \dfrac{h}{q_e}$. But either the model that the electrons move freely in an ideal ring [5], or the model that the electrons have hard-core interactions between them [6] can only give the sawtooth-type periodicity. Obviously, the sawtooth-type function is only the limit case for $q_e/\hbar \to 0$.

III. QUANTUM C-DESIGN AND COULOMB BLOCKADE

In Coulomb blockade experiments, the mesoscopic capacity may be relatively very small (about $10^{-8}F$) but the inductance of a macroscopic circuit connecting to a source is relatively large because the inductance of a circuit is proportional to the area which the circuit spans. We can neglect the term reversely proportional to L in (2), and study the equation for a pure C-design.

$$\left(\frac{1}{2C}\hat{q}^2 - \varepsilon\hat{q}\right)|\psi> = E|\psi>. \tag{7}$$

Apparently, the Hamiltonian operator commutes with the charge operator, so they have simultaneous eigenstates. The energy for the eigenstate $|n>$ is $E = (nq_e - C\varepsilon)^2/2C - C\varepsilon^2/2$, which involves both the charge quantum number and the voltage source. After some analyses, we find the relation between charge q and the voltage ε for the ground state,

$$q = \sum_{m=0}^{\infty}\left\{\theta[\varepsilon - (m + \frac{1}{2})\frac{q_e}{C}] - \theta[-\varepsilon - (m + \frac{1}{2})\frac{q_e}{C}]\right\}q_e \tag{8}$$

where $\theta(x)$ is the step function. The corresponding eigenstate is

$$|\psi(\varepsilon)>_{ground} = \sum_{-\infty}^{\infty}\left\{\theta[\varepsilon - (m - \frac{1}{2})\frac{q_e}{C}] - \theta[-\varepsilon - (m + \frac{1}{2})\frac{q_e}{C}]\right\}|m>. \tag{9}$$

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The dependence of the current on time is obtained by taking derivative

$$\frac{dq}{dt} = \sum_{m=0}^{\infty} q_e \left\{ \theta[\varepsilon - (m + \frac{1}{2})\frac{q_e}{C}] + \theta[\varepsilon + (m + \frac{1}{2})\frac{q_e}{C}] \right\} \frac{d\varepsilon}{dt}. \tag{10}$$

Clearly, the currents are of the form of sharp pulses which occurs periodically according to the changes of voltage. The voltage difference between two pulses are q_e/C. This is the called Coulomb blockade phenomena caused by the charge discreteness. If considering the problem in p-representation, we have

$$-\frac{\hbar^2}{2C} \left(\frac{d}{dp} - i\frac{C}{\hbar}\varepsilon \right) \tilde{\psi}(p) = (E + \frac{C}{2}\varepsilon^2)\tilde{\psi}(p). \tag{11}$$

Apparently, $\tilde{\psi}_\beta(p) \propto e^{i\beta p}$ solves the equation with the energy $E_\beta = \hbar^2(\beta - \frac{C}{\hbar}\varepsilon)^2/2C - C\varepsilon^2/2$, from which we know the ground state has $\beta = C\varepsilon/\hbar$. So the wave function for the ground state is $\tilde{\psi}_{ground}(p) = Ne^{i\frac{C}{\hbar}\varepsilon p}$ (N is the normalization constant).

REFERENCES

[1] F. A. Buot, *Phys. Rep.* 224(1993)73 and references therein.

[2] Y. Q. Li and B. Chen, *Phys. Rev. B*, 53(1996)4027.

[3] Y. Q. Li, *Commun. Theor. Phys.* 24(1995)255.

[4] V. Chandrasekhar, R. A. Webb, M. J. Brady, M. B. Ketchen, W. J. Gallagher and A. Kleinsasser, *Phys. Rev. Lett.*, 67(1991)3578.

[5] H. F. Cheung, Y. Gefen, E. K. Riedel and W. H. Shih, *Phys. Rev. B*, 37(1988)6050.

[6] Y. Q. Li and Z. S. Ma, *J. Phys. Soc. Jpn.*, 65(1996)1519.